A Thermodynamic Density Functional Theory of Static and Dynamic Correlation in Complex Alloys

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Objectives: Derive and implement a *thermodynamic DFT of structural ordering* in multi-component disordered alloys to obtain properties measured in diffuse scattering experiments.

Approach: Via *coarse-graining arguments*[1] in *KKR multiple-scattering theory*[2] we include *environmental effects* directly in configurational averaging and construct a first-principles *thermodynamic DFT of ordering* that is *systematically exact*.

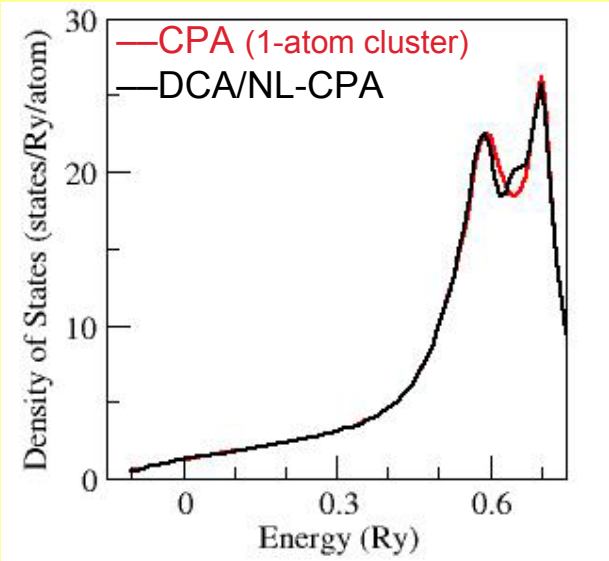
Significant Results: We have implemented the ***first*** *KKR-DCA/NLCPA code* and calculated electronic properties (e.g., *densities of states*, which exhibit important correlation that is missing in older single-site theories, *see Figure)*.

Current: We are validating our analytic formula for the **thermodynamic grand potential** that yields the required **systematically–exact electronic DFT**.

Broader Impact: Will permit ***direct calculation of structural transitions and correlations*** in strongly-correlated, size-mismatched, N-component alloys.

Example: KKR-based electronic density of states for disordered ***bcc NiAl* 1-atom** (***CPA,*** *coherent potential approx.*) and **8-atom cluster *DCA/non-local CPA***.

New electronic features arises from environmental correlations and will impact ordering.



D. Biava et al. (2004, to be published)

[1]M. Jarrell and H. Krishnamurthy. Phys Rev B 63, 125102 (2001)
[2]D Rowlands et al., Phys Rev B 67, 115109 (2003)